Modified BCS mechanism of Cooper pair formation in narrow energy bands of special symmetry
III. Physical interpretation

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In Part I of this paper a modified BCS mechanism of Cooper pair formation was proposed. The present Part III gives a physical interpretation of this mechanism in terms of spin-flipping processes in superconducting bands.

1. INTRODUCTION

In Part I of this paper [1] a modified BCS mechanism of Cooper pair formation was proposed that operates in narrow "superconducting" energy bands (σ bands) and can be established within a nonadiabatic extension of the Heisenberg model of magnetism [2]. This "nonadiabatic Heisenberg model" (NHM) is defined by three postulates given, e.g., in [3].

The present paper gives a physical interpretation of this mechanism. In Section 2 the special properties of the spin-dependent Wannier functions (spin-dependent Wfs) in narrow σ bands are interpreted in terms of spin-flipping processes. In Sections 3 and 4 the spin-phonon coupling in narrow σ bands and the resulting mechanism of Cooper pair formation, respectively, are illustrated in terms of these spin processes.

In Section 5 the important difference between the new mechanism in narrow σ bands and the conventional BCS mechanism [4] is interpreted in terms of "spring-mounted" Cooper pairs.

2. SPIN-FLIPPING PROCESSES

Assume a metal to be given that possesses a narrow, roughly half-filled σ-band complex in its calculated band structure. As in Part I we assume that this metal has only one atom in the unit cell. That means that the σ-band complex consists only of a single σ band.

The Bloch functions of the σ band can be transformed into spin-dependent Wfs $w_m(\vec{r} - \vec{T}, t)$ [as given in Eq. (A14) of Part I] with the following properties:

(i) they are centered on the atomic positions $\vec{T}$;

(ii) they are obtained by a *unitary* transformation from the Bloch functions of the σ band;

(iii) they are adapted to the symmetry of the considered metal; and

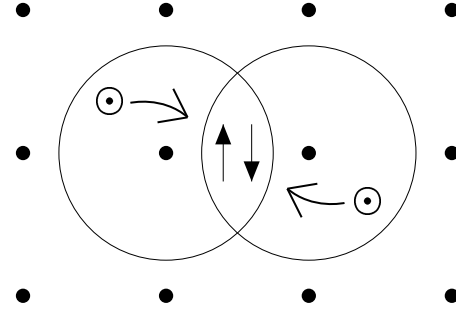(iv) they are as well localized as possible.

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FIG. 1: Spin-flipping process in a narrow σ band: two electrons with parallel spins (represented by small circles $\odot$) in adjacent localized states comply with the Pauli principle by aligning their spins antiparallel when they approach.

($m = \pm\frac{1}{2}$ is the quantum number of the crystal spin; $\vec{r}$ and t stand for the local and spin coordinate, respectively, of the electron.) However, the spin-dependent Wfs cannot be written as a product of a local function $w(\vec{r} - \vec{T})$ with the spin functions $u_s(t)$ (s denotes the spin quantum number) because the matrix $[f_{sm}(\vec{k})]$ in Eq. (A9) of Part I cannot be chosen independent of $\vec{k}$ in a σ band. Thus, these functions represent localized states $|\vec{T}, m\rangle$ with spin directions depending on the positions $\vec{r}$ of the electrons. This motion may be described in terms of "spin-flipping processes" as, e.g., illustrated in Fig. 1. Here two electrons with parallel spins align their spins antiparallel when they approach within the region of overlap.

It is essential that within the NHM the states $|\vec{T}, m\rangle$ are *really occupied by electrons*. This is a consequence of the second postulate of the NHM, i.e., of the special electron-electron interaction in the nonadiabatic system which is forced by this postulate. Hence, within the NHM the spin-flipping processes in a narrow σ band are produced by a *real electron-electron interaction* that operates in the nonadiabatic system.

The flippings of the spins are a consequence of the special mathematical properties of the spin-dependent Wfs $w_m(\vec{r} - \vec{T}, t)$ which are determined by the four above con-
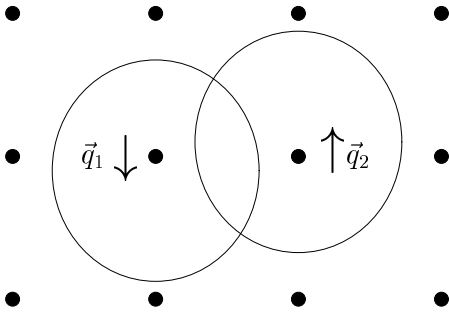
FIG. 2: The spin-flipping process indicated in Fig. 1 produces asymmetric charge distributions that accelerate the positive ions in such a way that a phonon pair is emitted or absorbed. $\vec{q}$ stands for the acceleration of the positive ions.

ditions (i) - (iv) that must be satisfied within the NHM. Hence, we understand the physical character of this interaction if we understand why the $w_m(\vec{r} - \vec{T}, t)$ must comply with these conditions.

The first and the fourth condition (i) and (iv) are required by the second postulate. Hence, these conditions allow the electrons to take the state of lowest Coulomb repulsion energy. The second condition (ii) yields a nonadiabatic Hamiltonian with the correct symmetry and the third condition (iii) guarantees that the spin-dependent Wfs are orthogonal. Hence, the third condition is required that electrons occupying the states $|\vec{T}, m\rangle$ comply with the Pauli principle.

Consequently, in the ground state of a narrow σ band *the electrons change permanently their spin directions in order to comply with the Pauli principle.*

3. SPIN-PHONON INTERACTION

In a narrow σ band, the operator $H_{\text{Cb}}^{n\sigma}$ of Coulomb interaction has the rather complicated form given in Eq. (3.13) of Part I. $H_{\text{Cb}}^{n\sigma}$ depends on boson as well as on fermion operators and represents a special "spin-phonon interaction" which may be understood as follows.

On a spin-flipping process as indicated in Fig. 1 the spin angular momentum of the two electrons is not conserved. During this process the electrons behave like gyroscopes: inertial forces act on the electrons that deform their orbitals within their localized states. As indicated in Fig. 2, the localized charge distributions become asymmetric with respect to the lattice and accelerate the positive ions in such a way that phonons are emitted or absorbed. Eq. (3.14) of Part I shows that $H_{\text{Cb}}^{n\sigma}$ conserves

the total crystal spin angular momentum.

4. COOPER PAIR FORMATION

As a consequence of the spin-phonon coupling in a narrow σ band, crystal-spin-1 phonons are excited in the ground state of the nonadiabatic system. We may assume that at zero temperature these phonons are virtually excited, i.e., each phonon pair is reabsorbed immediately after its generation. Therefore, in Part I we approximated the nonadiabatic Hamiltonian by a purely electronic Hamiltonian H^0 in order to describe the electron-phonon system at zero temperature; see Eq. (3.17) of Part I.

H^0 satisfies the equation of constraint (3.36) in Part I. This equation distinguishes the mechanism of Cooper pair formation within the NHM from the conventional BCS mechanism. As a consequence of this equation of constraint, in *all the eigenstates* of H^0 the electrons form Cooper pairs. This may be understood as follows.

The system represented by H^0 is purely electronic though the spin-flipping processes still occur. The electron spins still couple to the motion of the atomic cores and, hence, to the phonons. These phonons, however, *cannot store* crystal spin angular momenta but must be reabsorbed immediately after their generation. In this way, the phonons mediate a special spin-spin interaction between the electrons.

Thus, we have to look for a state with the total spin angular momentum being conserved within the electron system *alone.* That means, within the system represented by H^0 every spin-flipping process of two σ-band electrons must be accompanied by the opposite flipping process of two other σ-band electrons. This opposite process may occur somewhere in the crystal since the electron spins interact via virtual crystal-spin-1 phonons.

In this context, "opposite" means "time inverted" because the time-inversion symmetry is the only symmetry which makes such an opposite motion possible. Hence, the total spin angular momentum is conserved within the electron system if all the electrons form pairs that are invariant under time inversion. That means, whenever a certain one-electron state is occupied, then its time-inverted state must be occupied, too. In other words, all the electrons must form Cooper pairs.

5. CONSTRAINING FORCES

We obtain further information on the spin-flipping processes in a narrow σ band by transforming the operator $H_{\text{Cb}}^{n\sigma}$ of Coulomb interaction into the $\vec{k}$ representation,

$$H_{\text{Cb}}^{n\sigma} = \sum_{\vec{k},m} \langle \vec{k}_1'', l_1; \vec{k}_2'', l_2; \vec{k}_1, m_1, n; \vec{k}_2, m_2, n | H_{\text{Cb}} | \vec{k}_1', m_1', n; \vec{k}_2', m_2', n \rangle b_{\vec{k}_1'' l_1}^{\dagger} b_{\vec{k}_2'' l_2}^{\dagger} c_{\vec{k}_1 m_1}^{n\dagger} c_{\vec{k}_2 m_2}^{n\dagger} c_{\vec{k}_2' m_2'}^{n} c_{\vec{k}_1' m_1'}^{n} + \text{H.c.} \qquad (1)$$

with

$$\vec{k}_1'' + \vec{k}_2'' + \vec{k}_1 + \vec{k}_2 = \vec{k}_1' + \vec{k}_2' + \vec{K} \qquad (2)$$

where $\vec{K}$ stands for a vector of the reciprocal lattice. As already mentioned above, in addition $H_{\text{Cb}}^{n\sigma}$ conserves the crystal spin angular momentum. In bcc materials this conservation law may be expressed by the analogous equation [5]

$$l_1 + l_2 + m_1 + m_2 = m_1' + m_2' + 4n \qquad (3)$$

where n is an integer. The boson operators $b_{\vec{k}l}^{\dagger}$ and $b_{\vec{k}l}$ create and annihilate phonons with wave vector $\vec{k}$ and crystal spin $l = -1, 0, +1$; the fermion operators $c_{\vec{k}m}^{n\dagger}$ and $c_{\vec{k}m}^{n}$ create and annihilate nonadiabatic Bloch states with wave vector $\vec{k}$ and crystal spin $m = \pm\frac{1}{2}$.

Remember that $H_{\text{Cb}}^{n\sigma}$ depends on boson operators because during a spin-flipping process of two electrons a phonon pair is emitted (or absorbed) in a narrow σ band. Eq. (1) shows that these flipping processes are closely connected with scattering processes of the Bloch electrons: a flipping of two spins effects a scattering of these electrons within the $\vec{k}$ space or, vice versa, a scattering of two Bloch electrons effects a flipping of the spins.

The mechanism of Cooper pair formation via crystal-spin-1 phonons in a narrow σ band is characterized by the equation of constraint (3.36) of Part I. The physical origin of the related "constraining forces" may be understood as follows.

Assume all the N electrons (with N being even) in a narrow σ band to form (symmetrized) Cooper pairs of the form

$$\beta_{\vec{k}m}^{n\dagger} = c_{\vec{k}m}^{n\dagger} c_{-\vec{k}-m}^{n\dagger} - c_{\vec{k}-m}^{n\dagger} c_{-\vec{k}m}^{n\dagger}; \qquad (4)$$

cf. Eq. (3.25) of Part I. Two of these Cooper pairs are depicted in Fig. 3(a). The total crystal spin of each Cooper pair is zero.

Let be $\mathcal{P}^0$ the subspace of the Hilbert space spanned by the N-electron states in the σ band in which all the electrons form Cooper pairs. In $\mathcal{P}^0$ the electrons possess only $2N$ degrees of freedom because always *two* electrons are characterized by four quantum numbers k_x, k_y, k_z and m (cf. Section 4 of Part I). However, the electrons cannot stay in $\mathcal{P}^0$ because in reality they have $4N$ degrees of freedom. Thus, they necessarily become scattered out of this subspace creating then a phonon pair [satisfying Eqs. (2) and (3)] because any scattering process is connected with a flipping of the spins.

In Fig. 3(b) the two electrons with the wave vectors $\vec{k}_1'$ and $\vec{k}_2'$ become scattered emitting then a phonon pair
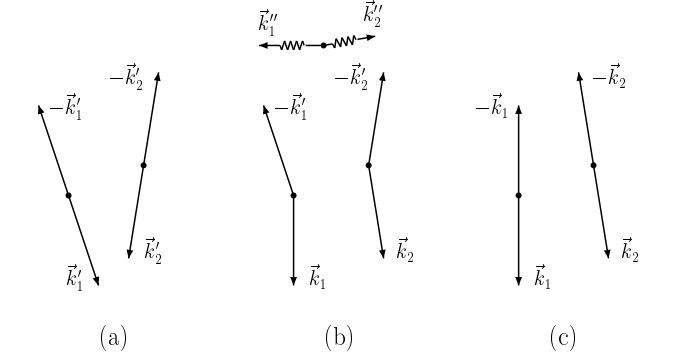

FIG. 3: "Spring-mounted" Cooper pairs in a narrow σ band:
(a) Four electrons form Cooper pairs. The total crystal spin of each Cooper pair is zero.
(b) The two electrons with wave vectors $\vec{k}_1'$ and $\vec{k}_2'$ are scattered on creating a phonon pair (with wave vectors $\vec{k}_1''$ and $\vec{k}_2''$). The total crystal spin of the four electrons *and* the two phonons is zero, while neither the four electrons nor the two phonons alone possess a defined total crystal spin.
(c) The two phonons can be completely reabsorbed only by the time-inverted scattering process. Hence, after the absorption of the phonons, the electrons again form Cooper pairs of zero total crystal spin.

with the wave vectors $\vec{k}_1''$ and $\vec{k}_2''$. The total crystal spin of the four electrons *and* the two phonons still is exactly zero (since $H_{\text{Cb}}^{n\sigma}$ conserves the crystal spin angular momentum), but the phonons and electrons are strongly coupled in the sense that neither the two phonons nor the four electrons *alone* possess a defined total crystal spin. The strength of this coupling as well as the wave vectors of the scattered electrons and the emitted phonons strongly depend on the special features of the preceding spin-flipping process. As stated above, the spins flip in a narrow σ band in order that the localized electrons comply with the Pauli principle. Hence, the features of the spin-flipping processes are determined by the wave vectors of the flipping electrons as well as by the wave vectors of all the other electrons that produce the potential in which the scattered electrons move.

The two phonons cannot be reabsorbed spontaneously because their complete absorption can only be the result of an appropriate motion of two other electrons in the σ band. Such a motion is given when these two other electrons are *forced by the Pauli principle* to change their spin directions in such a way that the phonon pair ($\vec{k}_1''$, $\vec{k}_2''$) is completely reabsorbed. Such a motion is performed by the time-inverted electron pair ($-\vec{k}_1'$, $-\vec{k}_2'$):

these two electrons carry out exactly the time inverted flipping process leading to a complete absorption of the phonon pair. Hence, after the absorption of the phonon pair the electrons again form Cooper pairs with zero total crystal spin, as illustrated in Fig. 3(c).

This mechanism may be interpreted in terms of "spring-mounted" Cooper pairs: There exist "springs" in the nonadiabatic system that push the electrons back into the subspace $\mathcal{P}^0$. These springs become tense when phonons get excited, and they become slacken again when these phonons are reabsorbed.

The operator H^0 represents a system with these springs being rigid. The effect of these rigid springs may be interpreted in terms of constraining forces that produce frozen Cooper pairs possessing half the degrees of freedom of unpaired electrons.

In analogy to classical physics, I suppose that only these quantum mechanical constraining forces produced by the described "springs" in narrow σ bands can produce stable Cooper pairs (with half the degrees of freedom of unpaired electrons). This supposition is corroborated by the calculated band structures of those metals that experimentally prove to be superconductors; see Part II of this paper [6].

Acknowledgments

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